Supplementary Data for

Hydroxylation Mechanism of Methane and its Derivatives over Designed Methane Monooxygenase Model with Peroxo Dizinc Core

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Table S1: Standard orientation of the species in the gas-phase reaction of Q + CH_3X (X = H, CH_3, CN, NO_2, F) calculated at the B3LYP/6-31G(d, p), Lanl2dz level

Q

O	-0.013488	-0.519776	-1.267597
Zn	1.671133	-0.806510	-0.245628
Zn	-1.680925	-0.833909	-0.225019
O	-0.014346	0.362827	0.054483
O	2.166954	-2.220099	1.210410
C	2.964257	-2.774910	0.392391
O	3.138290	-2.347635	-0.782428
H	3.524194	-3.661709	0.732614
N	2.994473	0.815860	-0.497330
C	2.553782	2.058475	-0.406623
N	3.569353	2.926636	-0.629004
C	4.717384	2.193395	-0.876557
C	4.340233	0.881080	-0.791376
H	1.524771	2.315118	-0.200046
H	3.497250	3.932534	-0.621761
H	5.665941	2.662237	-1.083460
H	4.923170	-0.017501	-0.922810
O	-2.139331	-2.250150	1.243085
C	-2.939665	-2.817237	0.436889
O	-3.132930	-2.396269	-0.737416
H	-3.485176	-3.709566	0.785980
N	-3.038200	0.761600	-0.471072
C	-4.384353	0.794862	-0.768663
C	-4.789573	2.097857	-0.867142
N	-3.658046	2.858116	-0.625192
C	-2.624515	2.014193	-0.392333
H	-5.747633	2.544118	-1.080105
H	-4.947378	-0.117679	-0.890266
H	-1.601369	2.295874	-0.189757
H	-3.607986	3.865379	-0.626277

QCH_4

O	0.147226	-0.099026	-0.983384
O	0.027593	0.455709	0.500425
Zn	1.700246	-0.707891	0.118375
Zn	-1.624709	-0.583046	-0.229066
O	2.058555	-2.289664	1.446727
C	2.873553	-2.786548	0.610649
O	3.113808	-2.246044	-0.505569
H	3.390088	-3.723257	0.876698
N	3.067514	0.899423	0.136924
C	2.607214	2.132597	0.259403
N	3.626234	3.018528	0.155473
C	4.796967	2.308429	-0.049334
C	4.429371	0.990660	-0.058774
H	1.562716	2.367868	0.406816
H	3.541298	4.022186	0.205387
H	5.753484	2.794129	-0.156689
H	5.031969	0.106676	-0.200036
O	-2.213176	-2.381844	0.642864
C	-2.963983	-2.621182	-0.354353
O	-3.069477	-1.830000	-1.331249
H	-3.544005	-3.558845	-0.352880
N	-2.958613	1.038395	-0.038720
C	-4.287333	1.174503	-0.383175
C	-4.705947	2.437178	-0.063949
N	-3.601165	3.068065	0.482010
C	-2.569172	2.191094	0.477854
H	-5.658516	2.931617	-0.166454
H	-4.826301	0.359462	-0.841161
H	-1.565751	2.386910	0.826304
H	-3.567557	4.015438	0.826349
H	0.181805	1.383009	2.789353
C	0.384111	1.843796	3.759062
H	0.421220	1.066008	4.524383
H	1.346038	2.362005	3.727988
H	-0.404859	2.558032	4.009880

QCH_4-TS1

O	0.028983	-0.568076	-1.232634
O	-0.010344	0.080230	0.876724
Zn	1.657054	-0.718169	-0.254611
Zn	-1.642024	-0.712760	-0.333912
O	2.407445	-2.114883	1.176110
C	3.266657	-2.492973	0.325179
O	3.358699	-1.984739	-0.828027
H	3.964943	-3.299326	0.608850
N	2.913839	1.020472	-0.242605
C	2.533860	2.241345	0.083938
N	3.556694	3.114044	-0.092365
C	4.648336	2.403293	-0.559311
C	4.230291	1.103150	-0.646891
H	1.549796	2.507934	0.437530
H	3.524226	4.106962	0.081280
H	5.591225	2.877732	-0.779137

H	4.760391	0.218877	-0.966171
O	-2.483162	-2.201276	0.930280
C	-3.305519	-2.496878	0.011768
O	-3.336203	-1.899011	-1.100220
H	-4.026143	-3.311725	0.199357
N	-2.898444	1.020416	-0.188174
C	-4.185224	1.166674	-0.663639
C	-4.628922	2.430418	-0.382741
N	-3.583588	3.053465	0.276237
C	-2.561701	2.167019	0.371858
H	-5.562179	2.931964	-0.582664
H	-4.680411	0.347114	-1.161575
H	-1.610499	2.366457	0.840930
H	-3.582096	3.998586	0.628085
H	-1.048268	0.341901	3.368572
C	-0.002239	0.357034	3.075200
H	-0.016201	-0.359510	1.855402
H	0.628576	-0.373248	3.581674
H	0.439659	1.342951	3.001878

QH

O	-0.000162	0.145040	1.123224
H	-0.000339	-0.128780	2.048571
O	0.000004	-0.904673	-1.413219
Zn	1.495139	-0.688496	-0.026644
Zn	-1.495451	-0.688219	-0.027081
O	2.323119	-2.229016	1.138436
C	3.166357	-2.500455	0.225558
O	3.218032	-1.876580	-0.865697
H	3.881322	-3.320190	0.413875
N	2.718590	1.054970	-0.097541
C	2.429078	2.191196	0.510686
N	3.433735	3.083469	0.334382
C	4.417495	2.475958	-0.426892
C	3.956833	1.213756	-0.685402
H	1.524962	2.368928	1.072896
H	3.461864	4.022368	0.701620
H	5.327266	2.985124	-0.701753
H	4.412274	0.400364	-1.229063
O	-2.323552	-2.228544	1.138427
C	-3.167078	-2.499536	0.225713
O	-3.218691	-1.875502	-0.865482
H	-3.882375	-3.318975	0.414037
N	-2.717966	1.055931	-0.097780
C	-3.956136	1.215695	-0.685519
C	-4.416088	2.478029	-0.426385
N	-3.431967	3.084613	0.335164
C	-2.427807	2.191689	0.511013
H	-5.325589	2.987832	-0.700959
H	-4.412071	0.402853	-1.229587
H	-1.523559	2.368566	1.073285
H	-3.459581	4.023333	0.702898

QCH_4-TS2

O	-0.081469	0.304262	-0.873375
O	2.369939	-0.045305	-0.589056
Zn	1.162340	1.685943	-0.328888
Zn	0.740074	-1.440079	-0.918839
O	2.540434	2.883428	-1.494351
C	1.776538	3.878226	-1.325021
O	0.714405	3.814390	-0.642766
H	2.051707	4.840463	-1.790351
N	1.175968	2.007362	1.805642
C	1.200722	1.100931	2.766582
N	1.013716	1.689698	3.973376
C	0.854511	3.047924	3.766209
C	0.956306	3.227742	2.413823
H	1.333350	0.038550	2.626404
H	0.972600	1.214511	4.862106
H	0.684702	3.737249	4.577599
H	0.873232	4.125381	1.820619
O	1.264163	-2.558147	-2.639129
C	0.230743	-3.277945	-2.478526
O	-0.574203	-3.119956	-1.520290
H	0.036652	-4.077987	-3.213905
N	1.377897	-2.610811	0.782500
C	0.808144	-3.761493	1.287228
C	1.654269	-4.318852	2.207570
N	2.756833	-3.483685	2.252332
C	2.552494	-2.470663	1.373162
H	1.581306	-5.207651	2.813752
H	-0.149478	-4.104705	0.927131
H	3.252420	-1.675598	1.161400
H	3.587641	-3.624703	2.806859
H	5.113283	-0.438441	-0.692959
C	4.668160	0.395950	-0.166051
H	2.713431	0.112356	-1.482586
H	4.566255	1.352484	-0.660946
H	4.617016	0.367885	0.914647

PCH_3OH

O	-0.541468	0.117306	-0.819830

Zn	1.221608	-0.203255	-0.270613
Zn	-2.059688	-0.181577	0.171020
O	2.381879	-1.968793	-0.303422
C	2.936918	-1.636368	-1.400093
O	2.699489	-0.557912	-1.996748
H	3.664959	-2.345505	-1.835824
N	2.518875	1.439712	0.314685
C	2.553921	2.056204	1.482122
N	3.448732	3.075169	1.449355
C	4.016939	3.104104	0.187776
C	3.427637	2.080341	-0.503352
H	1.968972	1.777370	2.345114
H	3.666157	3.693293	2.215895
H	4.768453	3.826738	-0.087317
H	3.592367	1.732932	-1.511677
O	-1.860268	-0.220369	2.428656
C	-2.694533	-1.173335	2.361932
O	-3.197379	-1.564461	1.270898
H	-3.000846	-1.681448	3.291266
N	-3.421775	1.102934	-0.881847
C	-4.728353	1.536941	-0.976526
C	-4.852592	2.363846	-2.059269
N	-3.590317	2.423226	-2.625155
C	-2.755783	1.651887	-1.891174
H	-5.694949	2.898222	-2.468729
H	-5.482648	1.226605	-0.269545
H	-1.696579	1.457912	-2.054107
H	-3.330759	2.941442	-3.450629
H	-0.060148	-0.319592	2.247880
O	0.881243	-0.464852	2.019487
H	1.464876	-1.517538	3.730124
C	1.319600	-1.671241	2.653003
H	0.601737	-2.486211	2.502191
H	2.261422	-1.959025	2.186450

P

O	0.000910	-0.002442	-0.427052
Zn	-1.464200	-0.876043	0.303434
Zn	1.463406	0.874321	0.304731
O	-1.973202	-2.959906	0.266044
C	-2.212716	-2.851143	1.503881
O	-2.091020	-1.755949	2.128983
H	-2.541066	-3.743396	2.062539
N	-3.057030	0.342583	-0.484196
C	-2.573878	1.325087	-1.231159
N	-3.585565	2.097445	-1.691288
C	-4.777183	1.582432	-1.211696
C	-4.428423	0.491217	-0.463371
H	-1.512887	1.453261	-1.414628
H	-3.480432	2.913492	-2.274801
H	-5.732056	2.028372	-1.439902
H	-5.063700	-0.188071	0.084266
O	2.085315	1.755559	2.131633
C	2.207633	2.850515	1.506294
O	1.970707	2.958489	0.267871
H	2.534160	3.743283	2.065196
N	3.058757	-0.341759	-0.482124
C	4.430496	-0.487245	-0.462316
C	4.781239	-1.577408	-1.211235
N	3.590460	-2.095016	-1.690143
C	2.577317	-1.325136	-1.229058
H	5.736983	-2.021052	-1.440275
H	5.064622	0.193366	0.085000
H	1.516444	-1.455307	-1.411956
H	3.486814	-2.910995	-2.274019

QCH$_3$CH$_3$

O	0.114916	-0.158433	-0.976619
Zn	1.788709	-0.686342	-0.027588
Zn	-1.584738	-0.578400	-0.034018
N	3.163971	0.913309	0.010397
C	2.782101	2.132490	0.348571
N	3.833052	2.983629	0.274411
C	4.943554	2.263707	-0.131209
C	4.508323	0.976519	-0.291438
H	1.770526	2.390058	0.625999
H	3.809125	3.969327	0.486602
H	5.909070	2.723755	-0.267398
H	5.047109	0.096198	-0.606586
O	0.140991	0.458105	0.490839
O	2.251422	-2.351452	1.146654
C	3.020115	-2.771833	0.227711
O	3.190885	-2.144495	-0.854737
H	3.558293	-3.719732	0.392491
O	-2.115865	-2.244383	1.122004
C	-2.944085	-2.586014	0.222857
O	-3.110437	-1.917769	-0.835872
H	-3.537562	-3.500751	0.385308
N	-2.842861	1.109868	0.076307
C	-4.190804	1.279574	-0.160979
C	-4.508260	2.602786	-0.018924
N	-3.321671	3.236073	0.309353

C	-2.342487	2.301542	0.353172
H	-5.439097	3.138631	-0.112779
H	-4.821829	0.442377	-0.416806
H	-1.298650	2.476797	0.569315
H	-3.201890	4.223491	0.476047
C	-0.018217	1.565236	3.747832
H	0.046108	1.064240	2.776236
H	-0.994065	1.318409	4.179035
H	0.752751	1.134971	4.395316
C	0.159780	3.079915	3.609100
H	1.138662	3.330849	3.183326
H	0.087022	3.590587	4.575644
H	-0.607580	3.514984	2.956781

QCH_3CH_3-TS1

O	-0.003345	-0.543302	-1.258485
O	-0.088209	0.296981	0.825074
Zn	1.587746	-0.550865	-0.205615
Zn	-1.651997	-0.657835	-0.303589
O	2.368106	-1.809810	1.342035
C	3.261914	-2.217509	0.540145
O	3.357257	-1.800264	-0.647006
H	3.986454	-2.967571	0.902316
N	2.804919	1.218644	-0.318967
C	2.382937	2.446203	-0.080560
N	3.371273	3.339752	-0.334353
C	4.483555	2.635762	-0.761071
C	4.112887	1.318303	-0.745615
H	1.392192	2.701153	0.263075
H	3.303431	4.341215	-0.236728
H	5.405846	3.126107	-1.028382
H	4.672033	0.432408	-1.005382
O	-2.434251	-2.034188	1.128012
C	-3.250221	-2.454921	0.253888
O	-3.306827	-1.983755	-0.916268
H	-3.942308	-3.268114	0.534679
N	-2.978100	1.031885	-0.355190
C	-4.263206	1.090639	-0.852485
C	-4.738070	2.368005	-0.725717
N	-3.713005	3.089029	-0.138438
C	-2.672196	2.243833	0.067285
H	-5.680506	2.820510	-0.989516
H	-4.735145	0.206554	-1.253185
H	-1.728390	2.517154	0.513704
H	-3.735756	4.069189	0.097609
H	-0.596047	1.567031	3.043922
C	-0.107649	0.599506	3.118691
H	-0.115427	0.000635	1.861891
H	-0.761305	-0.168108	3.539598
C	1.323902	0.583034	3.566559
H	1.796624	-0.382825	3.365951
H	1.909895	1.359496	3.066650
H	1.380211	0.769155	4.651026

QCH_3CH_3-TS2

O	-0.072363	0.296410	-0.800208
Zn	1.198307	1.659904	-0.292041
Zn	0.753730	-1.440150	-0.878875
O	2.412270	-0.071442	-0.537305
H	2.733627	0.071786	-1.440917
O	2.579081	2.835047	-1.488572
C	1.838259	3.844377	-1.303507
O	0.791867	3.801734	-0.596437
H	2.120544	4.800510	-1.777435
N	1.204221	1.989206	1.848980
C	1.143270	1.075500	2.801941
N	0.926685	1.663095	4.004246
C	0.836384	3.028544	3.802560
C	1.009039	3.213411	2.458029
H	1.233742	0.009241	2.657646
H	0.820938	1.183237	4.885123
H	0.657846	3.718612	4.611470
H	0.987520	4.117960	1.870018
O	1.301209	-2.530094	-2.612213
C	0.266677	-3.253935	-2.478386
O	-0.551421	-3.115166	-1.528794
H	0.083962	-4.040534	-3.231288
N	1.357981	-2.642055	0.812645
C	0.775957	-3.795203	1.297061
C	1.604898	-4.364053	2.225962
N	2.709615	-3.533234	2.296635
C	2.522828	-2.511466	1.423565
H	1.519079	-5.258201	2.822519
H	-0.176696	-4.131451	0.917746
H	3.227275	-1.715940	1.230934
H	3.529829	-3.681478	2.864769
H	5.149363	-0.415672	-0.812533
C	4.773133	0.463052	-0.299581
H	4.557568	1.339758	-0.899649
C	4.992808	0.630381	1.162523
H	5.943458	1.152441	1.366198
H	4.200275	1.235393	1.616141

H	5.046336	-0.327827	1.692129

PCH_3CH_2OH

O	0.551170	0.123904	1.989436
H	-0.403777	0.336071	2.039610
H	0.138869	-1.594701	3.091970
C	0.862239	-0.768906	3.073596
H	1.834635	-1.202395	2.834214
C	0.877812	-0.038022	4.409912
H	-0.101598	0.401941	4.627052
H	1.620567	0.766441	4.404516
H	1.127990	-0.728839	5.222777
O	-0.570121	-0.294285	-1.004890
Zn	1.109491	-0.483330	-0.193461
Zn	-2.191238	-0.269443	-0.139998
O	2.114266	-2.196335	0.529798
C	2.784423	-2.311555	-0.546577
O	2.691491	-1.510527	-1.508612
H	3.481649	-3.166575	-0.621453
N	2.477989	1.201151	-0.107668
C	2.458990	2.205782	0.749293
N	3.428617	3.103638	0.442897
C	4.103888	2.638892	-0.672264
C	3.499905	1.455384	-1.000059
H	1.780828	2.291261	1.584408
H	3.625704	3.953734	0.948280
H	4.929104	3.177573	-1.109860
H	3.722887	0.751584	-1.787158
O	-2.228808	0.428449	2.023188
C	-3.073735	-0.504478	2.173898
O	-3.467783	-1.231121	1.217712
H	-3.490105	-0.691555	3.177556
N	-3.392573	0.625838	-1.681070
C	-4.665518	1.012566	-2.048204
C	-4.645547	1.466634	-3.338501
N	-3.329524	1.346617	-3.751748
C	-2.605050	0.836493	-2.729324
H	-5.420469	1.851057	-3.982317
H	-5.500693	0.936493	-1.368674
H	-1.542161	0.600087	-2.706547
H	-2.966187	1.585168	-4.661901

QCH_3CN

O	0.011681	-0.745370	-1.187723
Zn	1.759771	-0.926307	-0.267545
Zn	-1.731523	-0.918787	-0.254397
O	0.013344	0.115827	0.150261
O	2.384056	-2.198020	1.301202
C	3.155790	-2.776740	0.478203
O	3.237386	-2.429722	-0.735016
H	3.779356	-3.611147	0.838543
N	2.951482	0.785720	-0.562711
C	2.440818	1.997535	-0.409811
N	3.393347	2.930792	-0.638000
C	4.572719	2.280123	-0.954933
C	4.279247	0.944855	-0.904183
H	1.416350	2.201527	-0.136150
H	3.258373	3.928299	-0.570884
H	5.482246	2.812805	-1.181503
H	4.913395	0.091266	-1.088567
O	-2.352243	-2.232194	1.276526
C	-3.129974	-2.788783	0.443450
O	-3.218579	-2.411613	-0.759856
H	-3.752149	-3.631236	0.787320
N	-2.965405	0.768669	-0.518792
C	-4.286957	0.860860	-0.906830
C	-4.657204	2.177584	-0.929888
N	-3.531592	2.885488	-0.547525
C	-2.533944	2.002557	-0.310106
H	-5.587543	2.663298	-1.176573
H	-4.860094	-0.023547	-1.139432
H	-1.537623	2.266667	0.011690
H	-3.458260	3.886804	-0.448782
H	-0.781486	0.855523	3.776647
C	0.084171	0.970379	3.118481
H	0.996551	0.894644	3.716391
C	0.032211	2.258877	2.435233
N	-0.010619	3.270653	1.864676
H	0.076520	0.173915	2.365182

QCH_3CN-TS1

O	0.001377	-0.030509	0.563419
H	0.000183	0.067312	1.744638
H	-0.910671	0.326327	3.377700
C	-0.001074	0.682319	2.893216
H	0.910592	0.331263	3.377393
C	-0.004918	2.083083	2.593553
N	-0.008072	3.200996	2.260353
O	0.001842	-1.166680	-1.236673
Zn	1.696886	-0.938393	-0.246762
Zn	-1.693507	-0.939327	-0.247348
O	2.580606	-2.104586	1.291531

C	3.377047	-2.587225	0.430989
O	3.353220	-2.246968	-0.786145
H	4.120337	-3.331213	0.762761
N	2.825029	0.835433	-0.568039
C	2.449356	2.063599	-0.250041
N	3.427726	2.944200	-0.567151
C	4.483247	2.239278	-1.116770
C	4.091971	0.928389	-1.109503
H	1.511516	2.337287	0.209312
H	3.390002	3.940177	-0.410753
H	5.386779	2.723031	-1.451360
H	4.614653	0.044184	-1.440823
O	-2.576327	-2.103657	1.293468
C	-3.371453	-2.589258	0.433469
O	-3.347216	-2.251655	-0.784446
H	-4.113936	-3.333608	0.766240
N	-2.825530	0.831864	-0.569591
C	-4.092445	0.920059	-1.112047
C	-4.488745	2.229413	-1.119451
N	-3.436384	2.938308	-0.568933
C	-2.454884	2.061458	-0.251138
H	-5.393870	2.709716	-1.454697
H	-4.611522	0.033846	-1.443678
H	-1.518800	2.339044	0.209404
H	-3.402656	3.934376	-0.412209

QCH$_3$CN-TS2

O	-0.004365	0.108184	-0.533055
Zn	0.970527	1.712361	-0.063319
Zn	1.015799	-1.525545	-0.718477
O	2.414988	0.132804	-0.477541
H	2.568033	0.326201	-1.419048
O	1.970302	3.074386	-1.380411
C	0.979018	3.859150	-1.283774
O	-0.025766	3.604693	-0.562243
H	0.999914	4.803127	-1.854572
N	1.222517	2.315924	1.971888
C	1.965264	1.830863	2.955335
N	1.767198	2.550490	4.085071
C	0.850971	3.548430	3.809150
C	0.522025	3.390349	2.491578
H	2.653882	1.000162	2.889579
H	2.228335	2.388357	4.967544
H	0.529653	4.258181	4.554266
H	-0.145090	3.962806	1.865570
O	2.008742	-2.235399	-2.475543
C	1.039799	-3.028254	-2.677312
O	0.050313	-3.110237	-1.896987
H	1.067689	-3.672449	-3.572633
N	1.327864	-2.858815	0.922042
C	0.686097	-4.083094	0.987777
C	1.051434	-4.722294	2.139832
N	1.929817	-3.865514	2.777019
C	2.071177	-2.756399	2.013323
H	0.777829	-5.679594	2.553256
H	0.029620	-4.400017	0.191992
H	2.721558	-1.932589	2.271844
H	2.404167	-4.035352	3.650996
H	4.768139	-0.670504	-0.804959
C	4.539641	0.129356	-0.111709
H	4.698091	1.152208	-0.430002
C	4.550307	-0.151616	1.256305
N	4.488230	-0.389081	2.404617

PCH$_2$CNOH

O	0.426949	0.007429	1.972589
H	-0.535676	0.190864	2.085067
H	0.111014	-1.328484	3.547569
C	0.910623	-0.743602	3.077274
H	1.667480	-1.439150	2.702251
C	1.510982	0.147659	4.090243
N	1.985734	0.878276	4.857275
O	-0.647568	-0.504573	-1.043282
Zn	1.032663	-0.551846	-0.223727
Zn	-2.280120	-0.365118	-0.211173
O	2.108419	-2.173458	0.628057
C	2.809508	-2.301302	-0.428462
O	2.686608	-1.553726	-1.428848
H	3.557855	-3.113854	-0.448536
N	2.328029	1.183182	-0.089751
C	2.320348	2.145339	0.817229
N	3.310672	3.035538	0.566278
C	3.990838	2.613514	-0.561728
C	3.367716	1.460817	-0.955662
H	1.642449	2.209215	1.654081
H	3.525793	3.846161	1.126749
H	4.833325	3.154787	-0.961406
H	3.594041	0.792073	-1.771612
O	-2.238689	0.306697	1.992630
C	-3.155605	-0.559182	2.125472
O	-3.619851	-1.213995	1.150364
H	-3.574038	-0.747344	3.127669

N	-3.398260	0.620818	-1.747636
C	-4.644753	1.086640	-2.114218
C	-4.585522	1.578610	-3.389227
N	-3.273481	1.400637	-3.793635
C	-2.588934	0.821223	-2.781379
H	-5.331395	2.023957	-4.028009
H	-5.490190	1.034670	-1.445256
H	-1.541745	0.526654	-2.759911
H	-2.888017	1.647876	-4.692440

QCH$_3$F

O	0.001154	-0.680036	-1.085640
Zn	1.728381	-0.914581	-0.132388
Zn	-1.726202	-0.914959	-0.132867
O	0.000921	0.128081	0.288753
O	2.379260	-2.307224	1.300845
C	3.155325	-2.811772	0.432947
O	3.233516	-2.369776	-0.747857
H	3.785165	-3.667129	0.728247
N	2.968074	0.774656	-0.381499
C	2.545219	2.012891	-0.183981
N	3.537405	2.888153	-0.475058
C	4.646753	2.168983	-0.883953
C	4.274127	0.854394	-0.819703
H	1.559274	2.286156	0.164139
H	3.469834	3.892223	-0.407980
H	5.568109	2.647043	-1.175379
H	4.833307	-0.037733	-1.056790
O	-2.376551	-2.305592	1.302956
C	-3.150953	-2.812931	0.435272
O	-3.228583	-2.373288	-0.746490
H	-3.779973	-3.668567	0.731519
N	-2.968748	0.772031	-0.382906
C	-4.274687	0.848299	-0.822118
C	-4.651232	2.161818	-0.885269
N	-3.544411	2.883901	-0.474695
C	-2.549914	2.011320	-0.183448
H	-5.573788	2.637399	-1.176945
H	-4.830986	-0.045270	-1.060573
H	-1.565256	2.287475	0.166025
H	-3.479947	3.888100	-0.406460
H	-0.896338	2.303918	3.226181
C	-0.001669	2.133910	2.620203
H	0.893801	2.305166	3.224645
H	-0.001297	1.127000	2.198533
F	-0.003230	3.062272	1.560150

QCH$_3$F-TS1

O	-0.000155	-1.067654	-1.162075
Zn	1.686359	-0.905150	-0.281785
Zn	-1.686684	-0.905210	-0.281631
O	-0.000395	-0.052811	0.756536
O	2.640364	-2.066768	1.231620
C	3.460182	-2.480664	0.357835
O	3.422867	-2.107407	-0.848734
H	4.240577	-3.196026	0.669521
N	2.808397	0.913677	-0.438851
C	2.465760	2.092132	0.051484
N	3.415520	3.013364	-0.245495
C	4.415838	2.384205	-0.964760
C	4.022628	1.078270	-1.073835
H	1.575026	2.293558	0.627604
H	3.395990	3.986028	0.020306
H	5.287203	2.910550	-1.319893
H	4.514382	0.240827	-1.544706
O	-2.640934	-2.066010	1.232364
C	-3.460981	-2.479883	0.358797
O	-3.423631	-2.107024	-0.847902
H	-4.241622	-3.194852	0.670768
N	-2.807862	0.914153	-0.439463
C	-4.022446	1.079114	-1.073659
C	-4.414400	2.385527	-0.965761
N	-3.412934	3.014613	-0.248031
C	-2.463755	2.092866	0.049221
H	-5.285576	2.912252	-1.320796
H	-4.515288	0.241588	-1.543246
H	-1.572328	2.294142	0.624324
H	-3.392275	3.987582	0.016564
H	-0.932643	0.635110	3.311842
C	-0.002757	0.865083	2.789902
H	0.922720	0.632667	3.318652
F	0.000686	2.159830	2.345291
H	0.000216	-0.220257	1.796967

PCH$_2$FOH

O	-0.267828	0.126839	0.695972
Zn	1.072504	1.272529	0.176241
Zn	-0.629383	-1.641554	0.261279
O	5.266010	-0.812374	0.851126
H	4.603036	-0.189888	0.454421
O	3.316555	0.853863	0.018761
C	3.227748	1.482627	-1.082721

O	2.143960	1.986334	-1.480513
H	4.125526	1.591380	-1.711983
N	0.664237	2.903218	1.504440
C	-0.384259	2.591726	2.257219
N	-0.670686	3.616050	3.092229
C	0.238197	4.634267	2.863024
C	1.060639	4.173386	1.871805
H	-0.900526	1.639685	2.166970
H	-1.424467	3.629174	3.762604
H	0.214261	5.563728	3.409070
H	1.898553	4.665644	1.402216
O	-1.721295	-2.677189	-1.279265
C	-2.467687	-3.112742	-0.355320
O	-2.288585	-2.820526	0.864508
H	-3.308477	-3.776162	-0.619083
N	1.186220	-2.755420	0.159900
C	1.585617	-3.687143	-0.779100
C	2.952350	-3.783563	-0.765925
N	3.380822	-2.899600	0.204214
C	2.293569	-2.299699	0.729486
H	3.637333	-4.383980	-1.342966
H	0.863754	-4.199725	-1.396428
H	2.354112	-1.548388	1.499608
H	4.325104	-2.585699	0.418136
H	6.230276	-1.032877	2.603481
C	5.338497	-0.545739	2.197709
H	5.342449	0.530710	2.409267
F	4.231678	-1.080006	2.873360

QCH_3NO_2

O	0.028664	-0.172614	-0.834382
Zn	1.761079	-0.564206	0.038527
Zn	-1.712660	-0.464227	0.074934
N	3.085993	1.071035	0.067658
C	2.740402	2.261656	0.531648
N	3.782110	3.118651	0.416203
C	4.844666	2.439339	-0.153339
C	4.394023	1.165074	-0.363183
H	1.776637	2.509120	0.953812
H	3.776081	4.086002	0.702115
H	5.792404	2.913550	-0.351435
H	4.901005	0.312262	-0.788026
O	0.059236	0.489676	0.609958
O	2.318216	-2.123517	1.345487
C	3.063047	-2.585264	0.428480
O	3.166447	-2.034057	-0.704610
H	3.642228	-3.500473	0.633005
O	-2.292328	-1.958259	1.447073
C	-3.082946	-2.415744	0.567463
O	-3.197201	-1.894704	-0.578889
H	-3.693238	-3.298999	0.816906
N	-2.898318	1.266316	-0.000853
C	-4.242006	1.437772	-0.266748
C	-4.560922	2.760594	-0.129127
N	-3.380904	3.391533	0.222730
C	-2.404749	2.458741	0.292222
H	-5.488513	3.297179	-0.246729
H	-4.867014	0.600785	-0.537771
H	-1.373986	2.652484	0.548059
H	-3.266851	4.370601	0.436373
C	0.159162	0.986713	3.576178
H	0.160889	0.344640	2.686812
H	-0.448859	0.560364	4.370462
H	1.177616	1.204028	3.893050
N	-0.473495	2.269568	3.151888
O	0.236405	3.100745	2.576894
O	-1.672018	2.415491	3.361226

QCH_3NO_2-TS1

O	-0.000039	-1.267037	-1.207995
Zn	1.688666	-0.991188	-0.217824
Zn	-1.689057	-0.991263	-0.218389
O	-0.000276	0.098500	0.416768
O	2.433474	-1.939720	1.526138
C	3.182364	-2.648023	0.786754
O	3.199288	-2.536390	-0.471984
H	3.844640	-3.387673	1.266414
N	2.973242	0.583554	-0.796467
C	2.783995	1.876557	-0.586583
N	3.836756	2.580286	-1.064122
C	4.745826	1.689403	-1.605777
C	4.194199	0.450581	-1.429636
H	1.940021	2.318106	-0.077905
H	3.941162	3.582158	-1.009096
H	5.672763	2.011715	-2.051996
H	4.575937	-0.523713	-1.693672
O	-2.434399	-1.941806	1.524100
C	-3.183282	-2.649122	0.783771
O	-3.200035	-2.535963	-0.474807
H	-3.845701	-3.389260	1.262479
N	-2.973151	0.584276	-0.795768
C	-4.194396	0.452395	-1.428605

C	-4.745388	1.691640	-1.603751
N	-3.835629	2.581660	-1.061837
C	-2.783094	1.877039	-0.585122
H	-5.672293	2.014763	-2.049450
H	-4.576745	-0.521515	-1.693167
H	-1.938665	2.317747	-0.076479
H	-3.939443	3.583553	-1.006131
H	-0.931099	0.787687	3.146745
C	0.000101	1.030818	2.644297
H	0.931104	0.787078	3.146826
H	0.000018	0.258246	1.559601
N	0.000547	2.393533	2.153628
O	-1.091234	2.933109	1.935374
O	1.092684	2.932277	1.935167

QCH_3NO_2-TS2

O	0.276806	-1.093308	0.784012
H	0.010122	-2.070608	0.844603
H	-0.894822	-1.683096	2.845194
C	-0.368385	-0.748568	2.954519
H	0.492789	-0.626340	3.593505
N	-0.973453	0.374368	2.547592
O	-2.023462	0.279696	1.768643
O	-0.526551	1.520997	2.827624
O	0.042318	-0.939766	-1.078177
Zn	1.912920	-0.620600	-0.617702
Zn	-1.697847	-0.648214	-0.097913
O	3.406788	-2.077680	-0.412369
C	3.921626	-1.681348	-1.501418
O	3.439899	-0.722380	-2.170654
H	4.824101	-2.193955	-1.871879
N	2.508813	1.265628	0.102324
C	2.016172	1.986725	1.100688
N	2.726113	3.131438	1.228860
C	3.720837	3.143674	0.268214
C	3.572300	1.975946	-0.426274
H	1.165127	1.739321	1.728090
H	2.548835	3.845976	1.918778
H	4.421110	3.957620	0.172084
H	4.135255	1.584213	-1.259600
O	-0.942866	-3.407020	0.960377
C	-2.065207	-3.395300	0.415692
O	-2.671448	-2.392821	-0.102873
H	-2.627986	-4.346407	0.368160
N	-2.797743	0.911117	-1.019656
C	-3.274371	1.085717	-2.304138
C	-3.923541	2.286505	-2.385767
N	-3.831236	2.843075	-1.123120
C	-3.147956	1.986976	-0.329145
H	-4.428646	2.781335	-3.199548
H	-3.118836	0.342873	-3.071425
H	-2.914557	2.139591	0.715079
H	-4.212857	3.730811	-0.833482

PCH_2NO_2OH

O	0.384068	0.022401	1.957664
H	-0.575564	0.238215	2.047592
H	0.073710	-1.238135	3.583237
C	0.838750	-0.657941	3.059660
H	1.679859	-1.296346	2.783886
N	1.384664	0.295488	4.141890
O	1.744599	-0.249359	5.177114
O	1.434675	1.497736	3.906029
O	-0.597469	-0.400680	-1.110557
Zn	1.079641	-0.557687	-0.306038
Zn	-2.229200	-0.345109	-0.266689
O	2.050831	-2.173596	0.700050
C	2.768802	-2.383314	-0.329665
O	2.685902	-1.689877	-1.374986
H	3.494675	-3.214763	-0.291130
N	2.413397	1.126386	-0.116700
C	2.422059	2.072033	0.809273
N	3.415684	2.958749	0.558561
C	4.077805	2.554973	-0.586708
C	3.442650	1.413298	-0.992263
H	1.767294	2.116971	1.667550
H	3.641566	3.758325	1.130498
H	4.916678	3.099525	-0.989481
H	3.654357	0.762614	-1.826670
O	-2.274202	0.295264	1.922467
C	-3.136423	-0.630264	2.041522
O	-3.533692	-1.316970	1.060828
H	-3.561659	-0.839085	3.036517
N	-3.393384	0.638950	-1.767008
C	-4.657589	1.078983	-2.103508
C	-4.632010	1.600948	-3.367636
N	-3.322374	1.467901	-3.796201
C	-2.606468	0.884778	-2.808092
H	-5.399689	2.040198	-3.984391
H	-5.490429	0.989385	-1.422865
H	-1.550641	0.623537	-2.809276
H	-2.957935	1.747383	-4.694324

Table S2: Vibration frequencies (cm^{-1}) scaled by a factor of 0.963 and IR intensities ($Debye^2$ amu^{-1} $Å^{-2}$) of the species in the gas-phase reaction of Q + CH_3X (X = H, CH_3, CN, NO_2, F) calculated at the B3LYP/6-31G(d, p), Lanl2dz level

Q

10/0.4, 25/0.8, 35/5.4, 38/1.1, 41/0.0, 50/0.0, 56/0.9, 63/10.0, 63/0.7, 68/0.1, 70/0.9, 117/11.6, 128/5.4, 132/0.1, 140/12.0, 165/8.7, 167/11.3, 187/0.1, 190/5.9, 211/10.9, 217/9.7, 252/19.9, 285/9.5, 312/53.8, 317/3.1, 325/84.9, 353/49.5, 375/93.0, 507/250.8, 545/10.5, 547/167.6, 624/3.0, 624/41.5, 656/0.5, 658/1.1, 715/5.0, 716/61.7, 754/0.9, 795/14.3, 796/64.6, 838/4.2, 845/42.0, 854/0.2, 855/1.3, 899/2.6, 899/23.0, 918/6.6, 919/9.2, 1026/0.4, 1026/0.2, 1033/54.1, 1038/124.4, 1068/24.8, 1069/4.8, 1110/12.3, 1114/13.7, 1153/11.0, 1154/1.6, 1233/8.1, 1234/4.5, 1294/19.5, 1294/50.7, 1335/3.8, 1335/17.4, 1347/53.7, 1348/144.5, 1407/34.0, 1407/4.3, 1474/13.0, 1474/52.0, 1529/21.1, 1530/17.3, 1585/166.4, 1593/554.6, 2923/57.1, 2924/180.3, 3167/47.4, 3169/1.7, 3170/2.4, 3170/14.3, 3188/1.0, 3188/1.5, 3541/1.3, 3541/157.7

QCH_4

5/0.5, 14/0.6, 15/0.3, 24/0.8, 29/0.1, 33/2.0, 37/3.8, 40/0.1, 48/0.4, 55/0.4, 59/0.4, 61/1.4, 63/9.7, 65/0.7, 70/0.4, 84/0.4, 111/0.8, 116/10.7, 128/2.7, 132/0.6, 138/16.2, 164/7.9, 168/11.2, 187/0.9, 190/4.0, 211/11.1, 217/8.7, 244/26.7, 283/8.9, 312/48.0, 318/2.8, 325/81.5, 342/56.1, 376/92.9, 503/241.2, 546/14.5, 549/160.6, 624/14.1, 624/31.2, 657/0.3, 658/1.2, 715/30.8, 717/35.0, 755/0.9, 795/29.2, 796/49.6, 838/16.0, 845/23.7, 856/9.9, 857/1.8, 899/6.4, 900/17.0, 918/6.9, 919/8.8, 1025/0.3, 1026/0.3, 1035/55.4, 1039/117.4, 1069/24.2, 1070/3.8, 1111/11.7, 1114/12.5, 1153/8.6, 1154/3.4, 1233/6.3, 1237/6.9, 1293/31.1, 1294/40.5, 1297/11.6, 1305/9.1, 1317/17.2, 1334/8.8, 1335/12.8, 1347/72.1, 1348/126.1, 1407/34.2, 1408/4.4, 1474/20.3, 1475/43.5, 1519/0.5, 1522/0.9, 1529/20.1, 1530/18.0, 1584/171.7, 1591/550.3, 2924/106.6, 2927/99.1, 2927/33.7, 3030/38.1, 3041/13.5, 3048/12.2, 3166/41.5, 3169/5.0, 3170/2.7, 3173/19.2, 3188/0.9, 3188/1.6, 3540/67.1, 3542/90.7

QCH_4-TS1

i781/289.5, 9/0.1, 19/0.7, 29/3.5, 34/2.4, 44/0.8, 46/1.4, 49/0.8, 50/0.1, 58/0.6, 65/0.1, 69/2.3, 78/4.0, 85/0.3, 90/0.1, 121/6.8, 124/5.5, 132/15.3, 134/0.5, 163/8.7, 165/8.1, 178/0.6, 185/1.7, 198/5.6, 204/23.4, 208/26.7, 236/1.2, 293/45.8, 295/20.8, 302/10.9, 313/95.0, 316/91.1, 426/27.7, 484/45.6, 535/34.3, 538/134.8, 588/8.6, 619/210.2, 624/9.6, 624/21.9, 655/0.1, 657/1.2, 715/8.2, 716/45.0, 723/32.6, 788/23.5, 789/56.6, 799/7.8, 807/23.9, 867/8.3, 871/8.2, 876/88.3, 895/4.2, 896/24.4, 918/5.1, 919/5.4, 1027/0.3, 1027/0.3, 1038/46.1, 1041/100.1, 1057/31.5, 1069/25.9, 1070/13.7, 1112/7.3, 1114/11.6, 1149/12.3, 1149/2.1, 1233/2.2, 1236/0.8, 1300/18.2, 1300/44.7, 1332/4.5, 1333/17.7, 1349/85.1, 1350/122.6, 1387/5.6, 1403/2.3, 1406/22.5, 1407/5.5, 1476/27.1, 1477/46.6, 1530/15.2, 1531/21.8, 1591/141.2, 1596/495.4, 2302/26.2, 2907/117.5, 2908/166.8, 2984/0.7, 3118/4.4, 3152/10.1, 3169/5.7, 3170/6.5, 3177/7.8, 3179/2.6, 3188/2.2, 3188/3.0, 3540/7.3, 3540/141.9

QH

10/0.1, 18/0.3, 36/5.8, 42/0.4, 46/0.8, 47/0.6, 53/0.5, 61/0.6, 68/7.2, 78/0.2, 85/0.4, 98/5.6, 116/1.7, 131/0.8, 136/9.3, 142/2.8, 155/5.5, 174/6.5, 177/15.0, 189/7.4, 201/9.6, 223/12.3, 304/50.9, 305/8.6, 309/68.4, 320/20.7, 340/7.1, 367/125.9, 395/181.3, 421/29.8, 523/76.6, 540/35.1, 544/134.3, 624/8.5, 625/39.0, 655/0.9, 658/2.3, 700/155.4, 717/5.5, 718/51.9, 787/28.2, 788/56.3, 812/14.5, 822/33.1, 865/0.8, 865/17.7, 896/4.1, 896/25.5, 918/4.7, 919/5.8, 1026/0.7, 1027/0.5, 1034/46.2, 1039/112.2, 1069/25.8, 1070/13.1, 1109/8.8, 1113/12.6, 1150/12.0, 1150/2.9, 1231/3.4, 1232/1.0, 1299/25.9, 1299/49.6, 1333/1.6, 1333/18.8, 1347/90.5, 1348/114.3, 1406/21.6, 1407/6.3, 1475/21.5, 1476/54.1, 1529/13.8, 1530/25.8, 1593/132.9, 1601/597.5, 2906/110.8, 2907/172.3, 3171/0.5, 3171/12.0, 3176/15.5, 3178/4.5, 3189/0.5, 3189/6.4, 3539/2.5, 3540/154.1, 3717/19.0

QCH_4-TS2

i280/161.8, 13/0.8, 23/0.7, 27/1.0, 31/0.2, 41/6.5, 49/0.4, 51/0.0, 57/0.2, 62/0.1, 66/3.1, 72/0.8, 87/1.9, 90/1.5, 102/2.6, 106/0.1, 115/1.0, 134/1.8, 142/14.0, 147/3.3, 157/6.9, 170/8.1, 183/2.2, 190/5.7, 196/6.1, 206/34.0, 226/6.8, 289/59.2, 300/8.0, 305/6.8, 311/121.8, 317/61.1, 380/1.2, 430/0.9, 449/13.2, 539/83.2, 545/55.2, 552/167.7, 624/16.6, 625/27.0, 655/1.6, 659/1.6, 663/73.9,

682/107.4, 716/28.9, 717/4.6, 720/51.4, 786/45.4, 788/42.5, 796/14.0, 831/25.2, 853/7.2, 871/7.3, 896/11.8, 896/11.3, 916/5.7, 918/3.7, 1026/0.2, 1028/0.1, 1040/62.8, 1046/80.5, 1069/17.3, 1074/18.8, 1113/6.3, 1118/12.6, 1147/8.9, 1148/2.8, 1236/4.2, 1243/0.5, 1299/29.9, 1301/34.8, 1329/16.1, 1331/5.1, 1348/118.4, 1351/100.3, 1369/4.6, 1388/3.2, 1405/13.8, 1408/14.6, 1472/31.2, 1480/37.6, 1526/10.4, 1531/22.0, 1592/101.8, 1595/517.0, 2906/166.1, 2909/134.7, 3016/5.7, 3168/6.0, 3170/22.1, 3170/9.9, 3171/9.8, 3182/8.8, 3188/2.4, 3189/3.0, 3194/1.4, 3537/69.8, 3539/79.7, 3662/50.8

PCH_3OH

14/2.7, 19/1.2, 39/3.3, 41/3.0, 50/0.3, 53/0.4, 61/0.6, 63/0.8, 76/0.3, 78/3.8, 88/3.8, 99/2.6, 106/1.4, 110/2.7, 116/15.3, 129/3.2, 135/6.8, 142/4.0, 146/7.0, 153/1.8, 164/17.5, 172/21.7, 175/8.4, 185/7.3, 196/11.9, 202/26.3, 249/12.9, 295/47.1, 302/63.2, 304/47.9, 319/45.9, 447/105.0, 534/89.4, 556/79.2, 624/26.0, 625/25.9, 657/4.2, 661/0.5, 709/36.9, 712/29.4, 719/164.2, 735/272.7, 782/32.7, 783/45.9, 818/19.9, 829/8.5, 863/10.5, 895/13.8, 899/23.8, 907/10.4, 910/9.7, 916/3.0, 1017/132.3, 1026/0.4, 1028/0.3, 1032/103.9, 1042/72.4, 1069/8.7, 1070/19.7, 1098/26.1, 1114/27.3, 1116/13.2, 1140/1.0, 1146/4.5, 1148/4.8, 1235/2.1, 1241/25.4, 1300/47.0, 1305/44.9, 1328/10.2, 1330/9.7, 1348/156.0, 1349/65.4, 1394/19.6, 1407/26.3, 1407/14.9, 1437/4.8, 1452/7.9, 1461/20.0, 1467/4.5, 1473/37.0, 1523/12.0, 1528/18.8, 1585/434.6, 1607/370.2, 2883/181.6, 2911/60.7, 2924/128.2, 2971/45.6, 3055/8.6, 3067/159.5, 3162/2.4, 3170/5.1, 3178/8.7, 3184/1.2, 3188/5.7, 3436/621.9, 3540/76.1, 3540/78.7

P

7/4.2, 13/3.7, 27/0.0, 40/0.1, 44/0.4, 45/0.8, 46/0.3, 54/0.2, 56/0.4, 76/0.6, 79/9.0, 112/0.0, 123/8.8, 137/14.4, 150/53.1, 168/2.0, 191/17.0, 193/9.0, 200/34.3, 210/3.8, 211/1.5, 290/1.9, 315/97.8, 317/10.3, 318/143.7, 421/48.7, 555/49.6, 556/112.0, 624/17.3, 624/36.3, 660/0.1, 660/0.2, 711/34.7, 711/42.2, 741/310.4, 795/40.7, 796/28.3, 830/7.6, 830/9.5, 880/7.7, 880/14.9, 898/27.2, 899/9.6, 912/12.8, 912/2.2, 1025/0.5, 1025/0.0, 1031/161.9, 1035/46.4, 1071/20.4, 1072/0.1, 1112/30.3, 1114/5.2, 1150/11.3, 1150/0.1, 1236/26.6, 1237/4.2, 1294/23.5, 1294/44.6, 1332/16.2, 1332/4.4, 1347/151.8, 1348/50.0, 1407/45.0, 1407/1.9, 1466/36.8, 1466/12.2, 1524/3.2, 1524/27.7, 1585/206.8, 1588/465.2, 2921/186.8, 2922/64.9, 3123/156.6, 3124/12.4, 3163/2.5, 3163/2.1, 3185/1.5, 3185/0.5, 3539/98.5, 3539/65.1

QCH_3CH_3

5/0.5, 10/1.0, 15/0.4, 18/0.0, 24/0.8, 33/3.4, 33/1.8, 40/0.3, 48/0.2, 50/0.5, 55/1.0, 62/4.1, 63/5.5, 66/0.7, 69/1.1, 79/0.2, 93/0.1, 116/11.6, 129/4.9, 132/0.2, 141/14.0, 164/8.0, 167/11.7, 188/0.0, 192/4.1, 212/9.8, 217/9.3, 243/27.2, 281/10.8, 312/39.0, 313/10.6, 317/3.1, 325/85.8, 346/50.6, 373/90.1, 508/239.6, 543/11.6, 547/167.7, 623/7.4, 624/36.0, 656/0.2, 658/2.0, 716/19.4, 717/44.4, 748/0.9, 795/16.9, 796/63.5, 797/4.1, 800/9.8, 837/6.4, 846/42.9, 853/2.3, 855/0.2, 899/2.0, 899/21.2, 918/6.1, 919/8.8, 966/0.1, 1026/0.4, 1026/0.2, 1034/49.4, 1038/116.1, 1069/26.7, 1070/4.7, 1110/8.7, 1114/10.5, 1153/11.3, 1154/1.7, 1179/0.5, 1183/0.0, 1233/7.5, 1235/4.1, 1294/18.7, 1294/51.4, 1335/6.1, 1335/15.0, 1347/55.9, 1348/145.6, 1365/0.2, 1389/0.5, 1407/32.5, 1407/5.8, 1458/0.4, 1462/0.8, 1462/5.4, 1470/9.7, 1474/15.5, 1475/48.3, 1529/22.7, 1529/16.4, 1584/163.6, 1591/555.6, 2919/32.2, 2925/66.8, 2926/167.1, 2934/21.3, 2970/28.6, 2981/25.0, 3005/62.2, 3009/35.0, 3169/5.7, 3169/4.7, 3170/41.6, 3173/9.8, 3188/1.3, 3188/1.2, 3541/22.8, 3541/132.0

QCH_3CH_3-TS1

i581/423.0, 14/0.0, 21/0.6, 31/0.9, 31/5.3, 39/0.5, 45/1.2, 51/0.3, 57/0.8, 60/0.7, 63/2.1, 69/2.6, 78/3.6, 84/0.3, 89/0.1, 120/6.7, 124/11.5, 130/4.9, 133/4.9, 148/5.8, 152/2.6, 165/9.5, 174/0.7, 182/3.0, 196/5.8, 199/18.9, 203/22.7, 232/7.5, 248/4.1, 288/43.8, 293/37.1, 307/38.3, 315/96.9, 372/75.2, 437/47.4, 535/26.4, 537/139.2, 602/183.1, 624/6.5, 624/20.3, 630/34.6, 656/0.4, 658/1.0, 667/9.0, 715/6.7, 716/49.9, 727/61.8, 787/25.4, 787/55.9, 803/8.3, 812/26.0, 832/8.0, 867/8.3, 869/8.1, 895/5.9, 896/21.3, 917/3.7, 918/5.7, 927/55.8, 1024/19.8, 1026/0.3, 1027/0.4, 1037/48.3, 1041/101.0, 1068/28.5, 1069/9.6, 1080/114.8, 1111/7.7, 1115/11.9, 1149/11.9, 1149/2.4, 1184/2.0, 1232/2.6, 1235/1.2, 1300/28.8, 1301/37.1, 1333/7.0, 1334/14.2, 1349/89.9, 1350/121.1, 1363/3.9, 1406/22.3, 1406/6.0, 1429/2.0, 1432/7.0, 1453/14.3, 1475/25.9, 1476/45.7, 1529/15.1, 1530/20.4, 1591/162.3, 1597/485.6, 2155/215.4, 2890/26.5, 2903/141.7, 2906/150.8, 2979/7.9, 2997/11.6, 3020/9.2, 3096/16.0, 3169/5.7, 3170/5.3, 3177/9.0, 3179/3.0, 3188/1.9, 3188/3.5, 3540/43.7, 3541/102.2

QCH_3CH_3-TS2

i214/16.6, 9/1.0, 21/0.7, 28/0.1, 35/3.8, 47/5.0, 49/0.5, 54/1.1, 61/0.7, 63/1.8, 68/0.7, 74/0.7, 85/1.0, 91/0.7, 95/2.0, 108/4.6, 117/0.2, 130/3.8, 133/5.9, 145/14.5, 158/8.2, 167/8.9, 175/1.5, 180/3.7, 190/3.3, 194/20.1, 198/19.9, 227/21.0, 249/1.8, 287/41.6, 298/11.7, 305/35.1, 309/131.9, 324/42.1, 464/45.3, 534/9.8, 537/81.5, 540/57.4, 554/132.4, 623/17.5, 624/14.5, 627/176.9, 655/0.7, 659/5.6, 715/31.3, 716/8.3, 718/32.5, 784/44.2, 786/48.8, 794/1.8, 795/19.9, 816/19.2, 819/15.4, 855/9.3, 868/6.7, 895/16.1, 895/5.3, 916/4.4, 917/3.2, 965/89.1, 1024/0.2, 1026/0.1, 1039/57.6, 1042/5.8, 1045/75.7, 1069/17.5, 1073/19.0, 1112/5.7, 1117/12.3, 1146/7.2, 1147/4.3, 1175/5.4, 1235/3.0, 1241/0.5, 1300/29.6, 1301/35.5, 1328/15.6, 1330/4.4, 1347/119.0, 1349/20.3, 1352/105.2, 1405/12.7, 1408/14.2, 1423/3.1, 1433/24.2, 1454/1.2, 1471/34.6, 1478/38.2, 1526/10.1, 1529/20.2, 1593/113.3, 1597/525.9, 2874/24.8, 2901/186.4, 2905/147.7, 2953/19.3, 2999/14.7, 3059/16.7, 3168/7.4, 3169/1.2, 3171/3.3, 3171/8.6, 3176/16.7, 3188/2.9, 3188/3.4, 3536/61.2, 3538/76.5, 3672/34.5

PCH_3CH_2OH

15/3.3, 16/0.1, 26/0.3, 37/2.0, 41/4.3, 49/0.9, 54/0.4, 59/0.5, 62/0.9, 70/0.4, 76/0.9, 83/6.8, 99/1.3, 103/7.8, 108/0.8, 120/3.2, 122/7.7, 132/3.9, 136/8.7, 146/1.9, 155/20.9, 168/25.4, 175/7.3, 184/6.4, 194/11.6, 202/28.8, 213/6.0, 279/1.0, 296/56.0, 302/58.0, 304/46.0, 319/42.1, 426/20.7, 447/101.9, 534/89.0, 556/79.0, 623/26.1, 625/25.6, 657/4.3, 660/0.5, 708/37.3, 712/28.3, 719/170.3, 734/257.3, 773/7.9, 782/31.8, 783/45.2, 821/20.5, 828/8.4, 860/15.3, 863/12.3, 895/13.5, 899/24.2, 906/10.2, 910/9.4, 916/3.1, 1026/1.2, 1027/138.2, 1028/1.7, 1032/84.9, 1041/74.9, 1069/3.4, 1070/17.5, 1073/54.6, 1103/5.5, 1114/25.2, 1115/15.5, 1146/4.6, 1148/4.5, 1235/1.7, 1241/27.1, 1254/19.3, 1301/47.1, 1305/43.7, 1328/10.3, 1331/9.7, 1346/74.6, 1348/88.4, 1350/52.0, 1375/17.2, 1404/31.3, 1407/25.3, 1407/13.4, 1450/3.1, 1453/1.8, 1461/19.8, 1473/36.7, 1474/4.0, 1523/12.0, 1528/18.5, 1585/442.5, 1606/383.4, 2883/181.1, 2924/87.8, 2926/50.2, 2930/22.4, 2997/14.2, 3003/36.4, 3030/27.5, 3067/163.1, 3162/2.4, 3170/5.3, 3179/9.2, 3184/1.2, 3188/6.1, 3442/565.4, 3540/84.8, 3540/69.2

QCH_3CN

14/0.0, 19/1.6, 22/0.6, 27/0.3, 34/1.5, 36/1.2, 38/1.6, 46/8.1, 52/3.6, 58/0.2, 63/8.5, 68/3.1, 70/2.7, 76/2.4, 87/6.1, 102/13.3, 117/14.3, 131/0.2, 132/6.4, 142/0.6, 145/19.6, 160/9.6, 166/8.7, 192/0.2, 195/2.4, 213/12.7, 214/7.4, 239/19.6, 266/15.8, 310/35.9, 316/23.8, 325/97.1, 355/51.8, 364/71.4, 385/1.8, 390/0.9, 528/247.2, 558/11.0, 562/154.3, 627/12.6, 628/48.3, 658/0.0, 660/1.4, 716/25.4, 718/42.2, 747/0.8, 795/23.3, 796/55.0, 844/2.2, 847/29.3, 853/2.9, 861/29.6, 894/2.9, 901/1.7, 901/14.0, 918/5.6, 920/8.6, 1022/10.7, 1026/0.2, 1026/0.2, 1031/3.4, 1039/45.5, 1043/111.3, 1071/20.4, 1072/4.3, 1112/4.2, 1116/11.0, 1154/10.1, 1155/2.4, 1235/2.7, 1237/4.9, 1294/23.2, 1294/45.9, 1331/9.1, 1332/12.1, 1348/64.1, 1348/140.5, 1362/9.5, 1409/35.3, 1410/9.3, 1420/4.1, 1433/17.6, 1476/23.7, 1478/44.1, 1529/20.6, 1530/17.8, 1583/130.2, 1590/577.7, 2267/24.3, 2927/90.6, 2928/144.5, 2933/30.8, 3010/18.2, 3027/1.2, 3168/2.2, 3168/2.9, 3176/79.5, 3181/15.7, 3188/2.4, 3188/1.9, 3539/19.8, 3539/149.6

QCH_3CN-TS1

i1278/291.9, 15/0.1, 16/1.3, 26/0.7, 37/1.5, 38/0.8, 39/2.1, 43/0.0, 51/10.4, 62/4.8, 72/1.7, 73/7.9, 74/2.6, 81/0.0, 84/1.5, 86/0.0, 110/10.5, 125/6.4, 138/1.0, 138/3.5, 167/7.7, 169/3.6, 185/0.1, 188/1.4, 196/23.9, 207/5.5, 210/21.4, 259/7.3, 294/37.5, 302/33.2, 313/30.0, 321/120.7, 345/39.2, 363/17.6, 381/20.9, 437/6.9, 444/7.9, 518/215.7, 552/28.0, 556/135.6, 626/8.4, 627/43.2, 636/1.0, 657/0.0, 659/1.6, 719/11.1, 720/53.6, 791/28.9, 792/55.0, 826/1.3, 836/35.4, 860/1.2, 860/12.9, 899/0.5, 899/14.7, 913/26.2, 918/4.7, 919/5.6, 943/2.8, 1003/22.7, 1027/0.3, 1027/0.3, 1042/37.7, 1044/99.8, 1073/21.4, 1074/9.0, 1113/4.7, 1116/7.0, 1133/46.5, 1151/12.7, 1152/2.3, 1236/0.5, 1237/0.7, 1292/72.9, 1297/11.6, 1297/41.8, 1329/5.3, 1330/16.7, 1348/88.4, 1349/121.7, 1398/5.3, 1409/26.7, 1409/10.6, 1478/20.1, 1479/53.7, 1530/17.6, 1531/18.9, 1586/105.5, 1591/551.7, 2223/34.3, 2921/105.6, 2921/153.6, 3001/1.1, 3080/0.3, 3170/0.3, 3170/8.4, 3175/43.9, 3179/12.1, 3189/0.9, 3189/3.0, 3538/0.8, 3538/161.7

QCH_3CN-TS2

i262/68.0, 14/0.1, 15/0.9, 35/2.8, 38/2.8, 47/0.6, 51/0.5, 57/1.3, 59/0.2, 66/0.1, 71/3.1, 73/5.9, 89/15.7, 96/1.1, 101/0.1, 105/7.8, 111/1.4, 124/3.8, 139/2.3, 149/23.7, 164/3.4, 165/10.1, 175/1.2, 185/0.0, 198/2.2, 200/3.4, 212/22.1, 241/12.2, 279/34.5, 298/37.7,

303/52.3, 312/76.4, 313/71.9, 385/2.5, 438/9.7, 480/3.1, 512/0.5, 551/37.8, 555/110.0, 562/149.9, 627/12.9, 627/36.6, 657/1.3, 659/1.8, 667/185.1, 720/21.2, 721/46.1, 737/56.1, 787/38.1, 788/51.6, 823/2.1, 836/3.3, 850/29.8, 867/4.9, 867/13.1, 898/1.2, 898/14.7, 917/5.1, 918/8.3, 1013/0.4, 1016/11.7, 1028/0.2, 1028/0.3, 1050/39.8, 1051/105.6, 1077/14.5, 1078/16.2, 1118/6.1, 1120/11.6, 1149/4.6, 1150/3.4, 1252/0.4, 1253/1.9, 1300/12.4, 1300/51.9, 1324/4.8, 1325/15.6, 1349/112.6, 1350/113.4, 1402/6.1, 1410/22.2, 1411/16.5, 1484/18.7, 1485/46.6, 1533/16.1, 1533/17.3, 1590/88.2, 1593/508.8, 2139/169.7, 2913/139.2, 2914/147.9, 3069/3.5, 3150/84.5, 3153/34.5, 3170/2.1, 3171/5.5, 3171/13.7, 3189/0.3, 3189/5.4, 3538/8.5, 3538/153.1, 3625/53.7

PCH_2CNOH

12/1.3, 15/1.6, 22/3.9, 36/2.4, 41/7.9, 48/0.8, 54/0.5, 55/1.4, 62/1.7, 72/0.8, 77/2.0, 86/2.8, 96/2.2, 102/4.4, 110/1.0, 117/23.0, 127/2.5, 134/8.9, 138/0.8, 150/2.0, 154/22.0, 167/26.4, 176/4.0, 185/4.7, 193/11.2, 204/29.1, 242/5.1, 259/21.2, 293/58.8, 301/43.2, 305/55.1, 324/55.0, 357/0.8, 445/100.1, 544/85.5, 560/78.9, 574/1.2, 624/27.0, 626/29.9, 657/4.1, 661/0.3, 711/26.9, 713/101.5, 715/24.5, 732/357.8, 781/43.7, 782/31.5, 817/23.2, 829/8.2, 854/10.1, 877/20.8, 896/11.1, 899/22.0, 903/11.2, 911/10.1, 917/2.7, 973/5.1, 1026/0.2, 1029/1.3, 1031/231.5, 1034/14.3, 1045/72.8, 1070/9.5, 1074/19.8, 1114/27.5, 1117/11.4, 1147/4.7, 1149/5.1, 1222/39.8, 1238/2.1, 1241/22.7, 1301/55.7, 1303/51.7, 1328/9.3, 1329/9.2, 1346/133.2, 1349/58.1, 1353/45.8, 1407/26.9, 1409/14.1, 1411/22.9, 1443/4.6, 1463/21.0, 1476/38.1, 1523/11.9, 1529/18.3, 1585/488.2, 1604/390.4, 2273/1.6, 2894/166.4, 2929/100.6, 2943/29.9, 3004/20.4, 3080/142.6, 3162/2.6, 3171/4.7, 3183/8.3, 3184/0.8, 3189/4.9, 3305/1061.1, 3539/83.7, 3539/81.5

QCH_3NO_2

13/0.1, 18/2.1, 24/0.2, 26/0.9, 33/0.9, 36/4.9, 37/2.5, 45/1.9, 50/0.3, 55/0.4, 61/2.5, 62/5.4, 71/1.6, 73/0.7, 87/3.8, 92/6.5, 110/6.8, 123/8.6, 134/3.9, 137/4.1, 152/29.4, 158/5.4, 168/8.3, 192/6.3, 194/0.1, 197/4.7, 215/9.4, 217/10.8, 238/21.0, 271/16.1, 310/36.3, 316/15.1, 326/94.1, 345/64.8, 366/71.0, 461/1.7, 528/228.8, 550/54.5, 558/117.5, 596/3.8, 623/18.6, 627/31.1, 639/20.7, 658/0.1, 659/2.9, 716/28.5, 717/39.4, 750/0.9, 795/25.3, 796/53.0, 845/0.4, 846/36.5, 853/0.6, 862/21.2, 898/8.6, 901/3.7, 902/12.9, 919/7.5, 920/8.2, 1026/0.3, 1026/0.2, 1039/63.3, 1046/90.8, 1072/14.8, 1073/8.7, 1081/14.5, 1107/5.2, 1113/6.0, 1119/13.1, 1154/8.0, 1155/3.7, 1235/4.1, 1244/4.2, 1293/25.6, 1294/43.2, 1331/10.2, 1332/9.7, 1348/63.7, 1348/145.2, 1365/27.4, 1396/63.8, 1409/32.3, 1411/7.9, 1425/47.6, 1427/8.0, 1479/23.3, 1480/44.7, 1530/21.0, 1531/21.4, 1582/131.2, 1589/490.9, 1594/363.6, 2927/129.7, 2928/62.8, 2929/124.7, 3047/18.5, 3103/1.1, 3165/87.1, 3168/2.8, 3168/6.9, 3178/18.3, 3188/1.0, 3189/1.2, 3540/74.0, 3542/94.7

QCH_3NO_2-TS1

i1199/130.5, 13/0.0, 16/2.4, 29/0.0, 36/0.1, 39/0.9, 40/1.1, 40/0.4, 41/6.1, 59/1.4, 64/2.5, 68/4.4, 80/0.8, 83/0.1, 84/0.4, 89/1.1, 110/16.7, 113/3.6, 125/4.7, 139/2.7, 140/3.7, 168/3.3, 169/7.2, 186/14.0, 191/0.0, 203/28.9, 211/23.8, 212/5.2, 271/13.0, 302/43.1, 305/32.3, 313/28.7, 322/100.0, 345/75.9, 379/20.4, 447/0.2, 495/5.2, 519/196.3, 520/1.0, 554/23.1, 556/131.3, 626/11.1, 627/46.4, 652/26.9, 656/0.9, 657/0.6, 716/29.2, 717/17.9, 719/30.0, 792/22.5, 792/62.1, 825/1.1, 831/36.5, 852/1.3, 852/12.8, 900/0.8, 900/11.5, 920/7.5, 920/8.0, 930/3.9, 979/34.0, 1019/12.8, 1027/0.3, 1027/0.2, 1047/58.4, 1048/86.9, 1075/13.5, 1076/10.6, 1111/97.9, 1118/0.5, 1119/9.5, 1153/9.3, 1153/2.3, 1246/0.6, 1247/1.3, 1297/12.2, 1297/55.1, 1329/3.9, 1329/6.2, 1348/72.6, 1348/218.1, 1358/241.6, 1388/76.9, 1398/16.2, 1411/36.3, 1411/8.8, 1483/23.9, 1484/49.8, 1532/49.8, 1533/28.6, 1548/292.2, 1585/114.2, 1590/521.7, 2922/82.5, 2923/169.1, 3036/1.3, 3151/0.3, 3170/0.2, 3170/7.1, 3172/66.8, 3174/19.7, 3189/1.1, 3189/2.2, 3539/9.9, 3539/159.5

QCH_3NO_2-TS2

i292/340.6, 15/1.9, 25/2.4, 28/2.7, 39/0.6, 47/0.5, 51/1.2, 62/2.3, 68/2.0, 77/1.1, 78/5.3, 84/1.2, 97/3.1, 107/0.7, 109/0.9, 116/5.3, 135/11.5, 140/10.9, 152/16.4, 163/19.7, 168/1.8, 185/9.8, 186/1.7, 196/2.8, 207/3.5, 214/33.6, 228/28.6, 253/0.0, 258/16.2, 309/82.5, 317/3.5, 326/120.6, 349/14.0, 385/47.3, 403/106.7, 522/1.6, 547/114.4, 557/93.2, 565/67.4, 625/28.2, 630/30.1, 638/5.7, 657/0.4, 659/0.1, 676/3.9, 715/36.1, 721/35.0, 729/3.5, 739/68.1, 757/130.2, 795/40.9, 833/9.4, 856/8.0, 864/12.6, 873/5.5, 901/9.9, 901/3.9, 918/7.0, 919/15.6, 971/45.9, 997/227.3, 1028/2.2, 1028/4.5, 1044/94.3, 1054/69.4, 1057/78.7, 1077/4.2, 1077/18.2, 1118/23.7, 1123/6.1, 1153/5.2, 1156/3.5, 1189/23.4, 1243/21.8, 1264/2.6, 1295/32.6, 1312/181.4, 1323/60.1, 1324/128.8, 1331/11.2, 1348/108.7, 1359/24.3, 1402/167.3, 1411/17.5, 1412/8.3, 1468/246.9, 1476/70.2, 1490/45.8, 1530/13.6, 1535/26.4, 1586/299.2, 1617/476.9,

2862/1353.0, 2892/138.0, 2931/126.4, 3077/199.5, 3097/10.5, 3165/6.5, 3167/35.8, 3170/6.5, 3188/0.3, 3189/1.2, 3229/4.0, 3538/75.7, 3540/99.2

PCH_2NO_2OH

15/1.7, 18/0.4, 31/1.0, 39/1.1, 43/5.6, 48/0.9, 55/0.9, 60/0.3, 64/1.0, 68/0.4, 75/1.0, 78/5.0, 85/7.8, 92/1.2, 97/2.4, 108/1.4, 113/7.6, 131/14.5, 135/5.1, 139/5.6, 156/11.9, 160/19.7, 169/21.2, 178/3.1, 185/4.1, 197/10.2, 205/28.3, 247/12.3, 290/58.0, 299/28.0, 307/50.3, 310/18.3, 326/68.5, 445/102.2, 486/12.6, 548/86.2, 556/7.3, 559/79.6, 624/27.3, 626/32.6, 658/6.2, 661/0.3, 667/44.0, 711/38.0, 714/26.9, 727/200.0, 757/284.6, 782/58.3, 784/30.3, 829/8.1, 842/33.0, 850/4.6, 853/5.9, 898/5.7, 899/18.6, 901/16.5, 911/9.5, 917/3.7, 1026/0.5, 1027/6.4, 1030/6.9, 1035/112.8, 1047/74.8, 1070/8.6, 1074/13.4, 1115/32.9, 1119/14.3, 1148/9.6, 1150/4.5, 1152/146.8, 1224/61.4, 1241/22.1, 1249/4.1, 1299/58.5, 1302/45.3, 1324/31.1, 1329/9.5, 1329/12.6, 1349/138.1, 1349/80.0, 1386/97.2, 1407/25.5, 1409/19.5, 1425/27.4, 1448/0.9, 1464/21.2, 1479/35.2, 1524/12.3, 1530/20.4, 1584/446.1, 1600/371.2, 1620/308.7, 2900/157.5, 2932/99.4, 2974/30.4, 3052/14.9, 3085/135.3, 3163/2.7, 3166/56.6, 3170/4.7, 3185/0.8, 3188/2.3, 3279/1078.0, 3539/94.6, 3539/72.1

QCH_3F

16/0.0, 20/1.1, 26/4.5, 31/0.4, 38/0.9, 43/0.9, 46/0.2, 53/0.0, 63/0.7, 64/0.9, 66/3.4, 75/0.0, 79/1.8, 87/3.7, 99/6.1, 103/13.9, 115/4.7, 128/2.0, 135/12.9, 136/0.5, 147/19.4, 163/8.8, 169/5.0, 188/0.0, 192/4.4, 212/9.7, 214/12.8, 240/25.0, 268/12.2, 310/38.9, 316/22.2, 324/96.3, 361/43.9, 366/76.3, 525/257.8, 549/16.1, 553/153.8, 625/5.0, 626/41.1, 660/0.0, 662/2.8, 717/8.6, 717/58.8, 745/0.7, 794/18.9, 795/60.4, 854/2.1, 854/20.7, 874/0.1, 888/44.3, 902/0.1, 903/18.8, 918/7.4, 919/10.1, 983/75.2, 1026/0.3, 1026/0.2, 1042/42.7, 1045/111.1, 1071/18.5, 1072/5.7, 1115/4.9, 1119/16.8, 1146/0.8, 1150/0.6, 1153/8.8, 1154/1.2, 1240/1.0, 1242/5.9, 1294/14.5, 1295/54.6, 1331/6.9, 1332/18.2, 1348/64.0, 1348/138.1, 1408/35.8, 1409/8.3, 1435/0.5, 1446/3.1, 1455/6.3, 1477/16.5, 1478/52.3, 1530/20.6, 1531/21.9, 1585/124.1, 1591/588.1, 2924/72.9, 2925/168.0, 2938/42.1, 3021/39.7, 3048/1.3, 3165/110.9, 3168/6.8, 3168/7.6, 3171/23.2, 3188/1.4, 3188/1.3, 3540/6.8, 3541/150.8

QCH_3F-TS1

i914/245.1, 12/0.0, 16/0.7, 22/0.0, 38/6.7, 40/0.2, 43/0.8, 54/0.0, 58/0.1, 63/0.1, 67/0.0, 74/0.4, 80/10.3, 87/0.4, 90/0.8, 107/4.5, 122/7.9, 124/5.7, 136/0.1, 147/14.7, 166/10.0, 182/14.6, 183/0.1, 190/12.3, 200/3.5, 202/25.7, 226/10.8, 288/50.7, 292/2.6, 301/32.9, 313/65.9, 316/108.3, 341/2.2, 423/20.1, 435/76.9, 541/40.7, 545/118.7, 593/44.0, 619/218.3, 625/2.3, 625/35.3, 658/0.0, 660/2.5, 717/14.5, 717/53.3, 789/30.5, 789/54.3, 824/52.9, 841/12.0, 852/39.0, 858/0.3, 860/3.2, 898/1.2, 898/17.7, 917/5.8, 918/11.2, 1013/336.3, 1027/0.2, 1027/1.4, 1044/38.9, 1046/111.0, 1071/17.6, 1072/7.3, 1092/41.5, 1116/6.1, 1119/16.4, 1149/7.2, 1150/2.2, 1176/12.7, 1243/2.2, 1245/2.3, 1300/12.1, 1300/51.4, 1331/4.0, 1331/15.8, 1348/98.5, 1349/112.5, 1407/24.2, 1408/10.4, 1430/1.4, 1478/17.0, 1479/52.3, 1530/14.7, 1531/21.4, 1590/102.7, 1594/525.6, 2503/25.1, 2910/130.1, 2910/154.6, 2970/9.3, 3090/13.0, 3169/0.2, 3169/8.3, 3174/42.8, 3177/12.4, 3188/0.9, 3188/3.8, 3540/0.9, 3541/146.6

PCH_2FOH

13/2.3, 21/0.6, 23/1.5, 27/1.7, 40/0.5, 45/0.3, 52/2.1, 55/0.4, 60/0.1, 69/0.4, 72/1.3, 79/1.6, 88/0.9, 98/3.8, 106/6.3, 113/4.6, 117/13.4, 132/21.2, 140/3.1, 150/30.6, 160/8.8, 175/9.4, 187/5.5, 199/16.4, 202/8.6, 218/3.8, 235/24.6, 289/15.7, 309/80.5, 312/25.9, 316/98.4, 435/95.3, 518/9.9, 560/78.9, 603/11.4, 624/29.0, 654/32.9, 660/0.1, 711/38.6, 718/6.9, 738/43.7, 748/370.7, 793/19.6, 794/34.4, 827/7.1, 834/18.8, 846/2.4, 882/96.1, 894/11.6, 900/18.8, 908/2.3, 911/9.2, 920/8.5, 970/206.9, 1026/0.2, 1026/0.2, 1034/125.2, 1051/47.2, 1071/9.0, 1075/34.9, 1084/6.4, 1115/21.2, 1123/147.2, 1132/49.9, 1150/4.6, 1164/10.1, 1233/5.0, 1240/24.1, 1242/4.9, 1296/33.1, 1300/60.9, 1327/16.0, 1329/10.6, 1348/111.9, 1353/84.9, 1401/22.6, 1408/25.4, 1421/23.7, 1465/23.3, 1473/24.9, 1483/12.6, 1490/40.5, 1524/9.3, 1525/34.1, 1589/324.5, 1594/520.7, 2918/146.4, 2931/80.0, 2934/94.2, 3002/81.5, 3096/124.7, 3162/2.9, 3165/1.2, 3185/0.8, 3185/0.5, 3200/11.1, 3207/1095.3, 3405/418.6, 3538/89.0

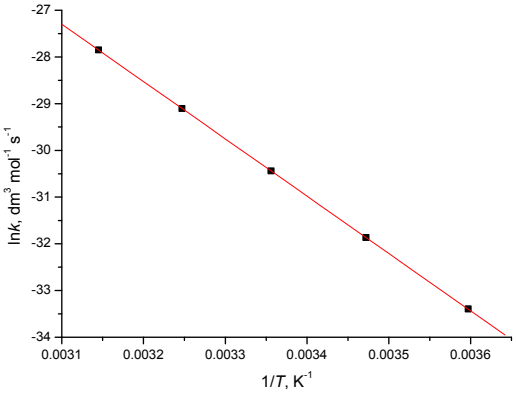
Table S3: Zero-point energies (*ZPE*) (hartree), total energies (E_c) (hartree) corrected by *ZPE*, and relative energies (E_r) (kJ mol^{-1}) for all the species in the reaction of Q + CH_3X (X = H, CH_3, CN, NO_2, F) calculated at the B3LYP/6-31G(d, p), Lanl2dz level in the gas phase, and the B3LYP/6-311++G(d, p), Lanl2dz level and the B3LYP*/cc-pVTZ, Lanl2tz level in the protein solution.

Species	B3LYP/6-31G(d, p), Lanl2dz in the gas phase			B3LYP/6-311++G(d, p), Lanl2dz in the protein solution			B3LYP*/cc-pVTZ, Lanl2tz in the protein solution		
	ZPE	E_c	E_r	*ZPE*	E_c	E_r	E_t	E_c (*ZPE* + E_t)	E_r
Q	0.20002	-1112.29721		0.19683	-1112.63069		-1106.17717	-1105.98034	
CH_4	0.04503	-40.47899		0.04437	-40.48971		-40.21031	-40.16593	
Q + CH_4	0.24505	-1152.77620	0.0	0.24120	-1153.12040	0.0	-1146.38748	-1146.14628	0.0
QCH_4	0.24566	-1152.77666	-1.2	0.24264	-1153.11781	6.8	-1146.38654	-1146.14390	6.3
QCH_4-TS1	0.24185	-1152.72349	138.4	0.23690	-1153.08139	102.4	-1146.34306	-1146.10617	105.3
QH	0.21015	-1112.94404		0.20686	-1113.28502		-1106.81596	-1106.60910	
CH_3	0.02977	-39.81311		0.02949	-39.82633		-39.54944	-39.51995	
QH + CH_3	0.23992	-1152.75715	50.0	0.23635	-1153.11135	23.8	-1146.36540	-1146.12905	45.2
QCH_4-TS2, $<S^2>$=0.751	0.24316	-1152.74894	71.6	0.24066	-1153.10108	50.7	-1146.36550	-1146.12484	56.3
PCH_3OH	0.25145	-1152.84495	-180.5	0.24826	-1153.19482	-195.4	-1146.45982	-1146.21155	-171.4
P	0.19720	-1037.15379		0.19233	-1037.47529		-1031.41577	-1031.22343	
CH_3OH	0.05141	-115.67256		0.04983	-115.72509		-115.04119	-114.99135	
P + CH_3OH	0.24860	-1152.82634	-131.6	0.24217	-1153.20039	-210.0	-1146.45695	-1146.21479	-179.9
Q	0.20002	-1112.29721		0.19683	-1112.63069		-1106.17717	-1105.98034	
CH_3CH_3	0.07493	-79.76381		0.07403	-79.78279		-79.24190	-79.16787	
Q + CH_3CH_3	0.27495	-1192.06102	0.0	0.27086	-1192.41348	0.0	-1185.41908	-1185.14821	0.0
QCH_3CH_3	0.27544	-1192.06111	-0.2	0.27196	-1192.41085	6.9	-1185.41777	-1185.14581	6.3
QCH_3CH_3-TS1	0.27075	-1192.01692	115.8	0.26593	-1192.38460	75.8	-1185.38346	-1185.11753	80.5
QH	0.21015	-1112.94404		0.20686	-1113.28502		-1106.81596	-1106.60910	
CH_3CH_2	0.05944	-79.10577		0.05873	-79.12721		-78.58879	-78.53007	
QH + CH_3CH_2	0.26959	-1192.04980	29.4	0.26559	-1192.41224	3.3	-1185.40475	-1185.13917	23.7
QCH_3CH_3-TS2	0.27330	-1192.02398	97.2	0.26946	-1192.40376	25.5	-1185.40634	-1185.13688	29.7
PCH_3CH_2OH	0.27990	-1192.13827	-202.8	0.27627	-1192.49661	-218.3	-1185.49882	-1185.22255	-195.2
P	0.19720	-1037.15379		0.19233	-1037.47529		-1031.41577	-1031.22343	
CH_3CH_2OH	0.08014	-154.96607		0.07823	-155.02722		-154.08092	-154.00269	
P + CH_3CH_2OH	0.27733	-1192.11985	-154.5	0.27056	-1192.50251	-233.8	-1185.49668	-1185.22613	-204.6
Q	0.20002	-1112.29721		0.19683	-1112.63069		-1106.17717	-1105.98034	
CH_3CN	0.04542	-132.71373		0.04486	-132.76026		-131.91940	-131.87455	
Q + CH_3CN	0.24544	-1245.01094	0.0	0.24169	-1245.39095	0.0	-1238.09658	-1237.85489	0.0
QCH_3CN	0.24661	-1245.02216	-29.5	0.24412	-1245.39101	-0.1	-1238.09851	-1237.85439	1.3
QCH_3CN-TS1, $<S^2>$=0.605	0.23939	-1244.99042	53.9	0.23633	-1245.36270	74.2	-1238.06160	-1237.82527	77.8
QH	0.21015	-1112.94404		0.20686	-1113.28502		-1106.81596	-1106.60910	
CH_2CN	0.03114	-132.06663		0.03075	-132.11217		-131.27572	-131.24497	
QH + CH_2CN	0.24129	-1245.01067	0.7	0.23760	-1245.39720	-16.4	-1238.09168	-1237.85408	2.1

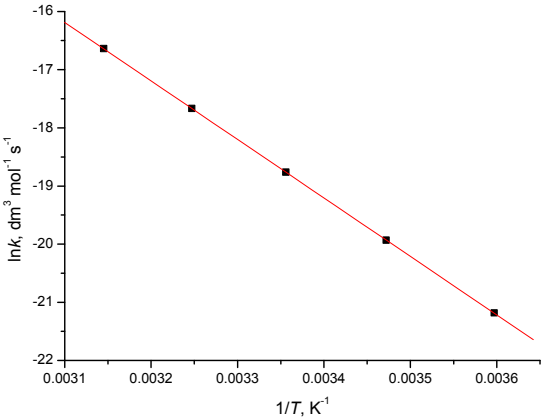
QCH_3CN-TS2, $<S^2>$=0.703	0.24493	-1245.01134	-1.0	0.24192	-1245.38979	3.0	-1238.09420	-1237.85228	6.9
PCH_2CNOH	0.25032	-1245.08121	-184.5	0.24703	-1245.46244	-187.7	-1238.16513	-1237.91810	-166.0
P	0.19720	-1037.15379		0.19233	-1037.47529		-1031.41577	-1031.22343	
CH_2CNOH	0.05038	-207.90546		0.04888	-207.99363		-206.74861	-206.69972	
P + CH_2CNOH	0.24758	-1245.05925	-126.8	0.24121	-1245.46892	-204.7	-1238.16437	-1237.92316	-179.2
Q	0.20002	-1112.29721		0.19683	-1112.63069		-1106.17717	-1105.98034	
CH_3NO_2	0.05001	-244.96337		0.04934	-245.05147		-243.66202	-243.61268	
Q + CH_3NO_2	0.25003	-1357.26058	0.0	0.24617	-1357.68217	0.0	-1349.83920	-1349.59303	0.0
QCH_3NO_2	0.25147	-1357.27273	-31.9	0.24794	-1357.68492	-7.2	-1349.84371	-1349.59577	-7.2
QCH_3NO_2-TS1, $<S^2>$=0.605	0.24425	-1357.24042	52.9	0.24066	-1357.65529	70.6	-1349.80587	-1349.56521	73.0
QH	0.21015	-1112.94404		0.20686	-1113.28502		-1106.81596	-1106.60910	
CH_2NO_2	0.03520	-244.30712		0.03492	-244.39775		-243.01197	-242.97705	
QH + CH_2NO_2	0.24535	-1357.25115	24.7	0.24178	-1357.68277	-1.6	-1349.82793	-1349.58615	18.1
QCH_3NO_2-TS2	0.25079	-1357.25413	16.9	0.24678	-1357.66952	33.2	-1349.82596	-1349.57918	36.4
PCH_2NO_2OH	0.25493	-1357.34510	-221.9	0.25097	-1357.76986	-230.2	-1349.92383	-1349.67286	-209.6
P	0.19720	-1037.15379		0.19233	-1037.47529		-1031.41577	-1031.22343	
CH_2NO_2OH	0.05519	-320.17345		0.05320	-320.29587		-318.50341	-318.45021	
P + CH_2NO_2OH	0.25238	-1357.32724	-175.0	0.24553	-1357.77116	-233.6	-1349.91917	-1349.67365	-211.7
Q	0.20002	-1112.29721		0.19683	-1112.63069		-1106.17717	-1105.98034	
CH_3F	0.03933	-139.69897		0.03889	-139.75604		-138.98983	-138.95094	
Q + CH_3F	0.23935	-1251.99618	0.0	0.23572	-1252.38673	0.0	-1245.16700	-1244.93129	0.0
QCH_3F	0.24090	-1252.00701	-28.4	0.23747	-1252.38771	-2.6	-1245.17090	-1244.93343	-5.6
QCH_3F-TS1	0.23586	-1251.95646	104.3	0.23124	-1252.35330	87.8	-1245.12953	-1244.89829	86.6
QH	0.21015	-1112.94404		0.20686	-1113.28502		-1106.81596	-1106.60910	
CH_2F	0.02481	-139.04283		0.02440	-139.09815		-138.33715	-138.31274	
QH + CH_2F	0.23496	-1251.98687	24.4	0.23126	-1252.38317	9.3	-1245.15311	-1244.92185	24.8
PCH_2FOH	0.24501	-1252.09722	-265.3	0.24132	-1252.48395	-255.3	-1245.26345	-1245.02212	-238.5
P	0.19720	-1037.15379		0.19233	-1037.47529		-1031.41577	-1031.22343	
CH_2FOH	0.04515	-214.91858		0.04319	-215.01532		-213.84557	-213.80238	
P + CH_2FOH	0.24234	-1252.07237	-200.0	0.23552	-1252.49061	-272.7	-1245.26134	-1245.02581	-248.2

Figure S1: Arrhenius plots of rate constants in the reaction of Q + CH_3X (X = H, CH_3, CN, NO_2, F) calculated at the B3LYP*/cc-pVTZ, Lanl2tz level in the protein solution

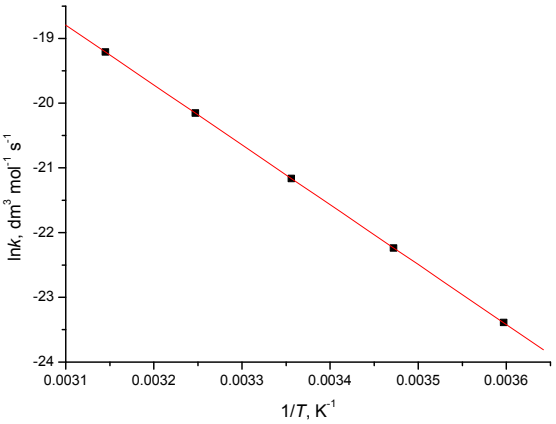
Reaction step of Q + CH_4 → QCH_4-TS1 → P + CH_3OH (k_1):



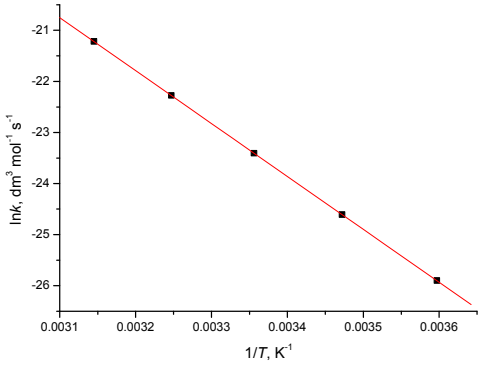
Reaction step of Q + CH_3CH_3 → QCH_3CH_3-TS1 → P + CH_3CH_2OH (k_2):



Reaction step of Q + CH_3CN → QCH_3CN-TS1 → P + CH_2CNOH (k_3):



Reaction step of Q + CH_3NO_2 → QCH_3NO_2-TS1 → P + CH_2NO_2OH (k_4):



Reaction step of Q + CH_3F → QCH_3F-TS1 → P + CH_2FOH (k_5)